Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1626gms

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

```
 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2  Apr 08  "Ask CAS" for self-help around the clock
 NEWS  3  Apr 09  BEILSTEIN: Reload and Implementation of a New Subject Area
 NEWS  4  Apr 09  ZDB will be removed from STN
 NEWS  5  Apr 19  US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
 NEWS  6  Apr 22  Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
 NEWS  7  Apr 22  BIOSIS Gene Names now available in TOXCENTER
 NEWS  8  Apr 22  Federal Research in Progress (FEDRIP) now available
 NEWS  9  Jun 03  New e-mail delivery for search results now available
 NEWS 10  Jun 10  MEDLINE Reload
 NEWS 11  Jun 10  PCTFULL has been reloaded
 NEWS 12  Jul 02  FOREGE no longer contains STANDARDS file segment
 NEWS 13  Jul 22  USAN to be reloaded July 28, 2002;
                  saved answer sets no longer valid
 NEWS 14  Jul 29  Enhanced polymer searching in REGISTRY
 NEWS 15  Jul 30  NETFIRST to be removed from STN
 NEWS 16  Aug 08  CANCERLIT reload
 NEWS 17  Aug 08  PHARMAMarketLetter(PHARMAML) - new on STN
 NEWS 18  Aug 08  NTIS has been reloaded and enhanced
 NEWS 19  Aug 09  JAPIO to be reloaded August 18, 2002

 NEWS EXPRESS  February 1 CURRENT WINDOWS VERSION IS V6.0d,
               CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:14:36 ON 13 AUG 2002

Golam Shameem

```
=> FIL REGISTRY
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:14:47 ON 13 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:   12 AUG 2002  HIGHEST RN 443729-39-3
DICTIONARY FILE UPDATES:  12 AUG 2002  HIGHEST RN 443729-39-3

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Calculated physical property data is now available.  See HELP PROPERTIES
for more information.  See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s isoflavones?
L1             0 ISOFLAVONES?

=> s isoflavones
               0 ISOFLAVONES
L2             0 ISOFLAVONES

=> s flavones
L3             1 FLAVONES

=> s flavone?
L4          6194 FLAVONE?

=> FIL CAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    17.52      17.73

FILE 'CAPLUS' ENTERED AT 10:17:21 ON 13 AUG 2002
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Golam Shameem

FILE COVERS 1907 - 13 Aug 2002 VOL 137 ISS 7
FILE LAST UPDATED: 12 Aug 2002 (20020812/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

```
=> s l4
L5        28254 L4

=> s l5 and isoflavones
          2454 ISOFLAVONES
L6        1459 L5 AND ISOFLAVONES

=> s l6/proc
          28254 L4
              1 ISOFLAVONES/CT
        3189134 PROC/RL
              0 ISOFLAVONES/PROC
                  (ISOFLAVONES/CT (L) PROC/RL)
L7            0 ((L4) AND ISOFLAVONES/PROC)

=> s l6/prep
          28254 L4
              1 ISOFLAVONES/CT
        2897488 PREP/RL
              0 ISOFLAVONES/PREP
                  (ISOFLAVONES/CT (L) PREP/RL)
L8            0 ((L4) AND ISOFLAVONES/PREP)

=> s l5/proc
FIELD CODES CANNOT BE CHANGED HERE
You may have tried to apply a field code to a term that already has a
field code.  You can only add a field code to a term that has no field
code appended to it.

=> log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              14.47      32.20

STN INTERNATIONAL LOGOFF AT 10:26:40 ON 13 AUG 2002
```

Golam Shameem

(130)

09/889,701

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1626gms

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:31:56 ON 13 AUG 2002

Golam Shameem

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:32:15 ON 13 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3
DICTIONARY FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

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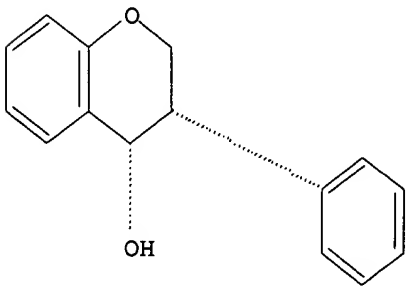
Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09889701.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

Golam Shameem

```
=> s l1
SAMPLE SEARCH INITIATED 09:32:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    604 TO ITERATE

100.0% PROCESSED     604 ITERATIONS                          11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        10606 TO    13554
PROJECTED ANSWERS:              21 TO      417

L2            11 SEA SSS SAM L1

=> FIL CAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                0.38       0.59

FILE 'CAPLUS' ENTERED AT 09:32:42 ON 13 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 13 Aug 2002  VOL 137 ISS 7
FILE LAST UPDATED: 12 Aug 2002  (20020812/ED)

  This file contains CAS Registry Numbers for easy and accurate
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CAS roles have been modified effective December 16, 2001. Please
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information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> s l1
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 09:32:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    604 TO ITERATE
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100.0% PROCESSED 604 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 10606 TO 13554
PROJECTED ANSWERS: 21 TO 417

L3 11 SEA SSS SAM L1

L4 8 L3

=> s l3/prep
8 L3
2897488 PREP/RL
L5 5 L3/PREP
(L3 (L) PREP/RL)

=> s l3/proc
8 L3
3189134 PROC/RL
L6 0 L3/PROC
(L3 (L) PROC/RL)

=> s l5 and hydrogenation
147967 HYDROGENATION
1893 HYDROGENATIONS
148239 HYDROGENATION
(HYDROGENATION OR HYDROGENATIONS)
L7 2 L5 AND HYDROGENATION

=> d ibib abs hitstr l7

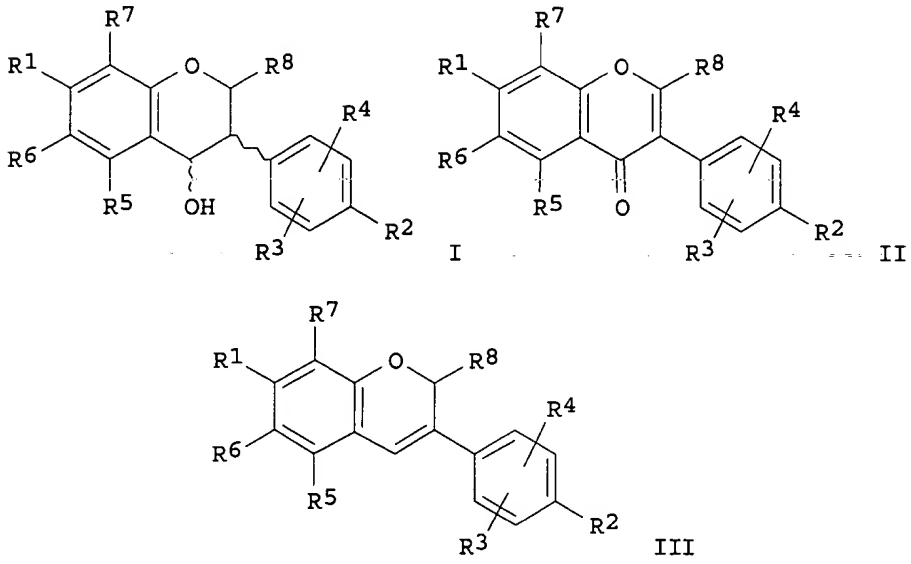
L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:592710 CAPLUS
DOCUMENT NUMBER: 133:177059
TITLE: Preparation of isoflavone derivatives
INVENTOR(S): Heaton, Andrew; Kumar, Naresh
PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000049009	A1	20000824	WO 2000-AU103	20000215

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

Golam Shameem

BR 2000008222 A 20011030 BR 2000-8222 20000215
EP 1153020 A1 20011114 EP 2000-904727 20000215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
NO 2001003945 A 20010814 NO 2001-3945 20010814
PRIORITY APPLN. INFO.: AU 1999-8685 A 19990215
WO 2000-AU103 W 20000215
OTHER SOURCE(S): MARPAT 133:177059
GI



I II III

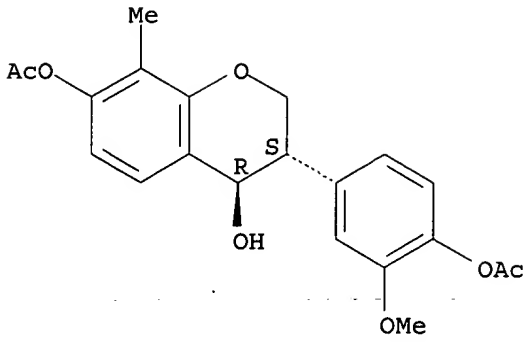
AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH2, NO2, alkyl, haloalkyl, aryl, arylalkyl,alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prepd. Thus, daidzein diacetate was prepd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the **hydrogenation** of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

IT **288266-89-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **288266-88-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
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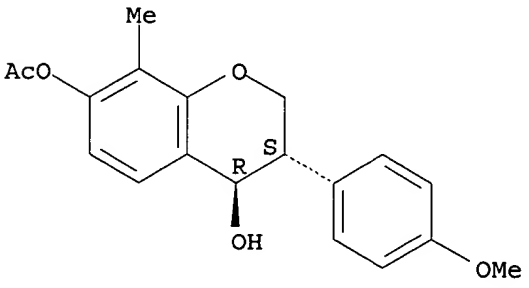
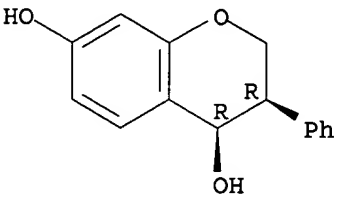


IT **288267-21-0P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of isoflavone derivs.)
RN 288267-21-0 CAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr l5

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
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DOCUMENT NUMBER: 133:177059
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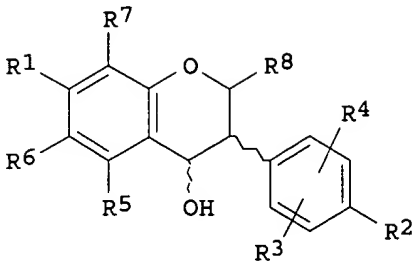
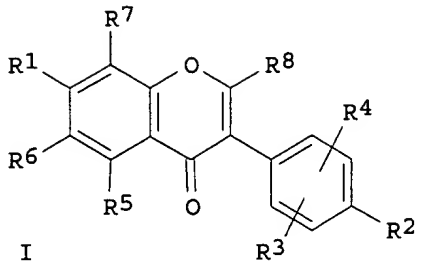
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000008222	A	20011030	BR 2000-8222	20000215
EP 1153020	A1	20011114	EP 2000-904727	20000215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
NO 2001003945	A	20010814	NO 2001-3945	20010814

PRIORITY APPLN. INFO.: AU 1999-8685 A 19990215
WO 2000-AU103 W 20000215

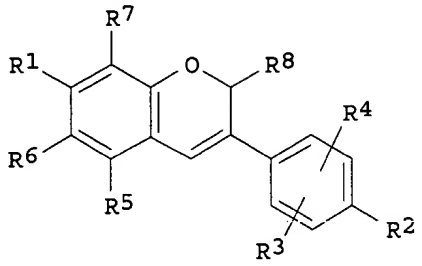
OTHER SOURCE(S): MARPAT 133:177059
GI



I



II



III

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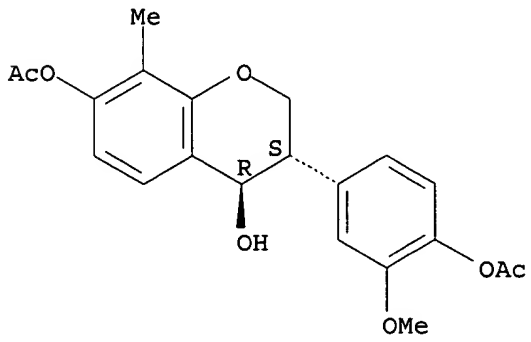

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RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or

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RN 288266-88-6 CAPLUS
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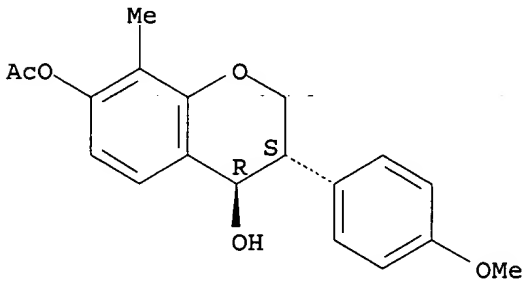

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(prepn. of isoflavone derivs.)
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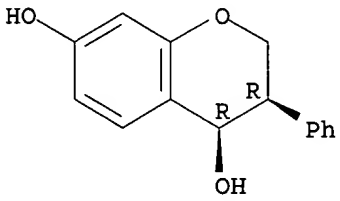
Relative stereochemistry.



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=> d ibib abs hitstr l5 tot

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DOCUMENT NUMBER: 133:177059
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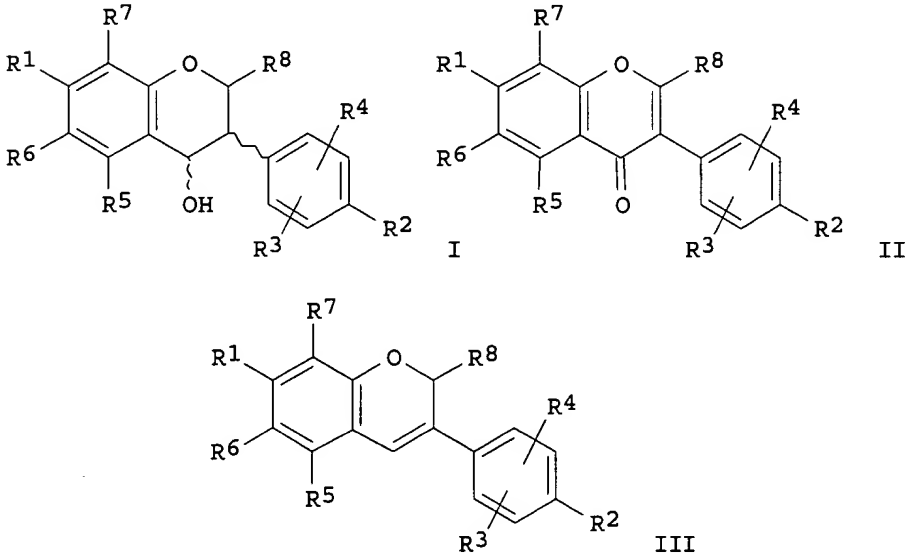
INVENTOR(S): Heaton, Andrew; Kumar, Naresh
PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2000049009 A1 20000824 WO 2000-AU103 20000215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
BR 2000008222 A 20011030 BR 2000-8222 20000215
EP 1153020 A1 20011114 EP 2000-904727 20000215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
NO 2001003945 A 20010814 NO 2001-3945 20010814
PRIORITY APPLN. INFO.: AU 1999-8685 A 19990215
WO 2000-AU103 W 20000215
OTHER SOURCE(S): MARPAT 133:177059
GI



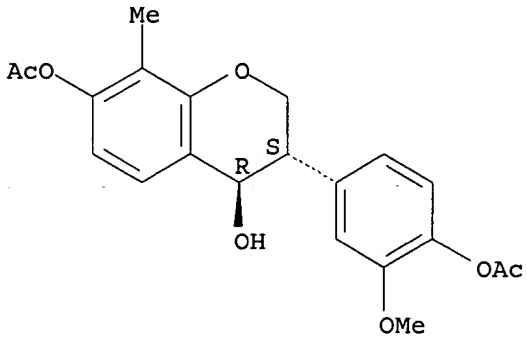
AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH2, NO2, alkyl, haloalkyl, aryl, arylalkyl,alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prepd. Thus, daidzein diacetate was prepd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the hydrogenation of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

IT **288266-89-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

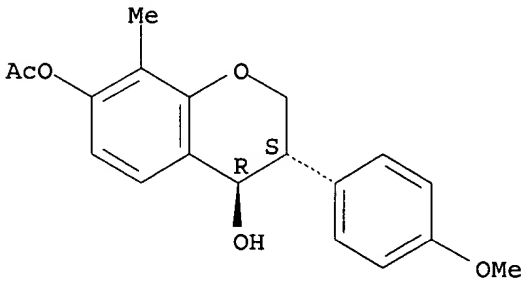
CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



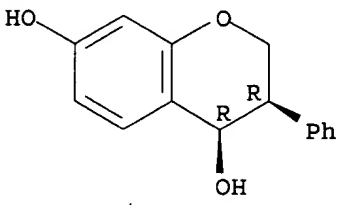
IT **288266-88-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(prepn. of isoflavone derivs.)
RN 288266-88-6 CAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **288267-21-0P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of isoflavone derivs.)
RN 288267-21-0 CAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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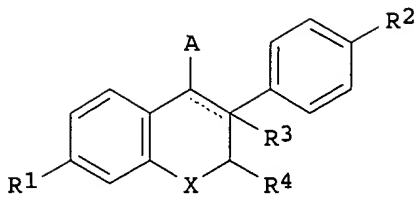
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

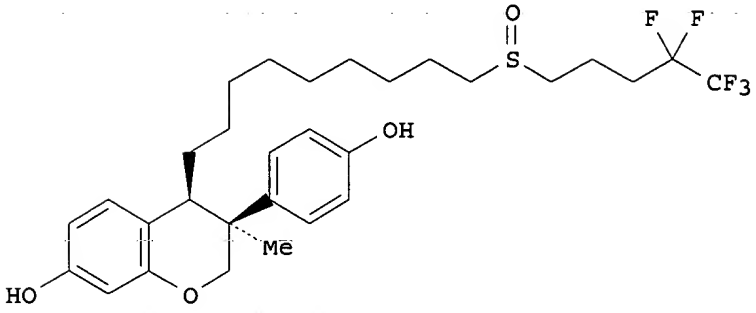
L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:402432 CAPLUS
DOCUMENT NUMBER: 129:81667
TITLE: Novel benzopyran and thiochroman derivatives useful as antiestrogens
INVENTOR(S): Jo, Jae Chon; Park, Sung Dae; Lim, Hyun Suk; Kim, Ju Su; Kim, Sung Jin; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myung-hwa
PATENT ASSIGNEE(S): C & C Research Laboratories, S. Korea; Jo, Jae Chon; Park, Sung Dae; Lim, Hyun Suk; Kim, Ju Su; Kim, Sung Jin; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myung-Hwa
SOURCE: PCT Int. Appl., 125 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825916	A1	19980618	WO 1997-KR265	19971213
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9854134	A1	19980703	AU 1998-54134	19971213
AU 722089	B2	20000720		
EP 944613	A1	19990929	EP 1997-947971	19971213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1244863	A	20000216	CN 1997-181472	19971213
JP 2000507620	T2	20000620	JP 1998-526521	19971213
JP 3251946	B2	20020128		
US 6153768	A	20001128	US 1999-319616	19990608

PRIORITY APPLN. INFO.: KR 1996-65301 A 19961213
KR 1997-26915 A 19970624
WO 1997-KR265 W 19971213
OTHER SOURCE(S): MARPAT 129:81667
GI



I



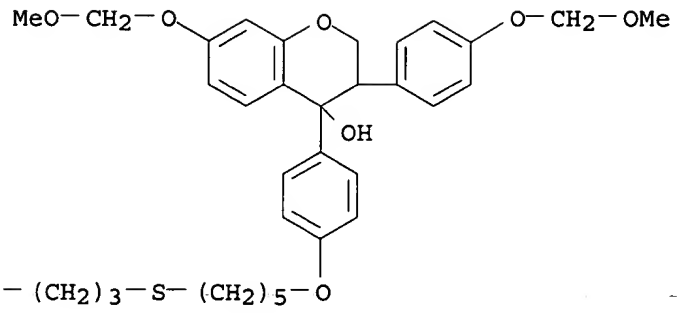
II

AB The invention relates to novel benzopyran derivs. having anti-estrogenic activity. More specifically, the invention relates to novel benzopyran and thiochroman derivs. I and pharmaceutically acceptable salts thereof [in which the dashed line = optional pi bond; R1, R2 = H, OH, or OR; R = acyl or alkyl; R3 = H, alkyl, haloalkyl, or null when R3 is absent; R4 = H or alkyl; A = (CH2)mSOnR5, C6H4O(CH2)mSOnR5, C6H4O(CH2)mNR6R7, (CH2)mSOn(CH2)pNR6R7; R5, R6, and R7 = H, alkyl, haloalkyl, alkenyl, or haloalkenyl; or NR6R7 = 4- to 8-membered heterocyclic ring which can be substituted with R5; X = O, S, or NR8; R8 = H or alkyl; m = 2-15; n = 0-2; and p = 0-4]. Also disclosed are a prepn. process, and antiestrogenic pharmaceutical compns. which contains I as an active component. Examples include over 80 syntheses and 4 bioassays. For example, compd. II was prepd. by a 7-step sequence involving: (1) double-O-methoxymethylation and 3-methylation of 7-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-4H-benzopyran-4-one (66%), (2) 4-alkynylation with HC.tplbond.C(CH2)7OSiMe2CMe3 (100%), (3) desilylation (33%), O-tosylation (88%), thioetherification (97%), deprotection of OH groups (66%), and S-oxidn. with NaIO4 (73%). The antiestrogenic and MCF-7 cell growth-inhibiting activities of II were comparable or superior to the related antiestrogen ZM-189154, and the side effect of decreased bone mineral d. in II was not only reduced but to some extent reversed.

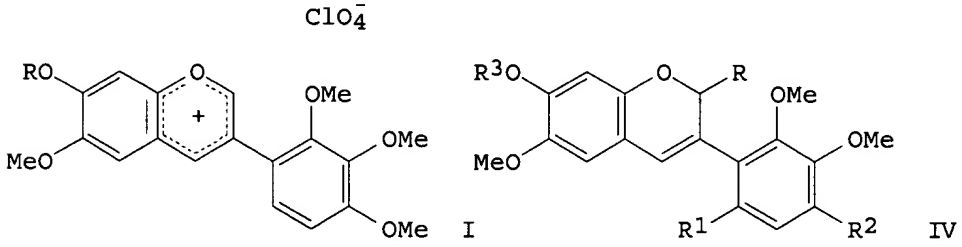
IT **209324-98-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of benzopyran and thiochroman derivs. as antiestrogens)

RN 209324-98-1 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-7-(methoxymethoxy)-3-[4-(methoxymethoxy)phenyl]-4-[4-[[5-[(4,4,5,5,5-pentafluoropentyl)thio]pentyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

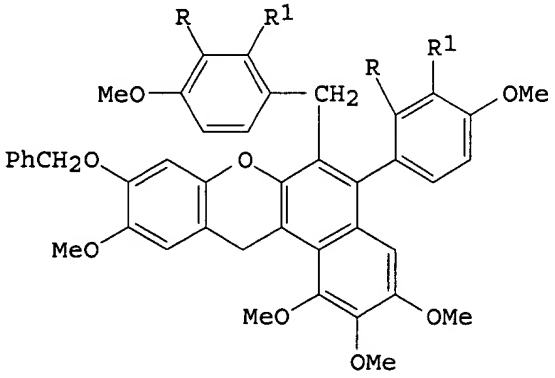


L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:148589 CAPLUS
DOCUMENT NUMBER: 104:148589
TITLE: The chemistry of the 'insoluble red woods'. Part 16. Some further observations on the condensation of isoflavylium salts with 1,3-diphenylpropenes
AUTHOR(S): Afonya, Theophilus C. A.; Epelle, Faithwin B. M.; Osman, Soad A. A.; Whalley, W. Basil
CORPORATE SOURCE: Sch. Pharm., London, WC1N 1AX, UK
SOURCE: J. Chem. Res., Synop. (1985), (10), 305
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:148589
GI



I

IV



V

AB Condensation of isoflavylium perchlorate I (R = CH2Ph) (II) with

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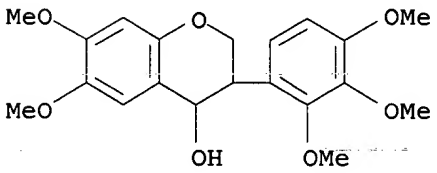
3,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-2,4 (III) in refluxing MeCN for 3 h gave isoflavene IV (R = R1 = H, R2 = OMe, R3 = CH2Ph) and benzoxanthene V (R = H, R1 = OMe). Similar reaction of II with 2,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-3,4 (VI) gave isoflavene IV (R = R2 = OMe, R1 = H; R = R2 = H, R1 = OMe; R3 = CH2Ph) and benzoxanthene V (R = OMe, R1 = H). Analogous reaction of I (R = Me) with III or VI gave only the isoflavene IV (R = R2 = OMe, R1 = H, R3 = Me). The prepns. of the starting materials are reported.

IT **100753-48-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and elimination reaction of, isoflavylium salt by)

RN 100753-48-8 CAPLUS
CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-6,7-dimethoxy-3-(2,3,4-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

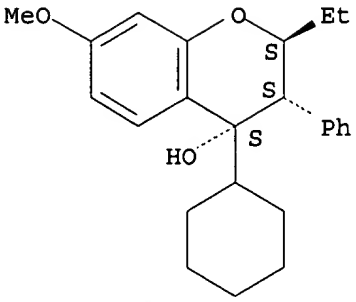


L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1971:476524 CAPLUS
DOCUMENT NUMBER: 75:76524
TITLE: Reactions of isoflavanones with Grignard reagents. Synthesis of estrogenic and antiestrogenic active isoflavanoids
AUTHOR(S): Irmscher, Klaus; Borck, Joachim
CORPORATE SOURCE: Chem. Forsch. E. Merck, Darmstadt, Ger.
SOURCE: Justus Liebigs Ann. Chem. (1971), 744, 164-77
CODEN: JLACBF
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Grignard reaction of isoflavanones or 2-ethyl-7-methoxyisoflavanones (I) gave 4-aryl-4-isoflavanols or 2-ethyl-7-methoxy-4-aryl-4-isoflavanols (II), resp., which were dehydrated to 4-aryl-3-isoflavenes. Depending on the reaction conditions, the constitution of the isoflavanone, and the Grignard reagent, the C-2 atom of the isoflavanone was also attached in some cases to give .beta.-aryl-.alpha.-phenyl-2-hydroxypropiophenones with ring opening. The mechanism of the ring opening involving an .alpha.-methylene ketone was discussed.

IT **33103-17-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

RN 33103-17-2 CAPLUS
CN 4-Isoflavanol, 4-cyclohexyl-2-ethyl-7-methoxy-, stereoisomer (8CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1967:28657 CAPLUS
DOCUMENT NUMBER: 66:28657
TITLE: 3,4-Diaryl-4-chromanols and 3,4-diaryl-3-chromenes
PATENT ASSIGNEE(S): Merck, E., A.-G.
SOURCE: Neth. Appl., 26 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6517021		19660704		
PRIORITY APPLN. INFO.:			DE	19650102

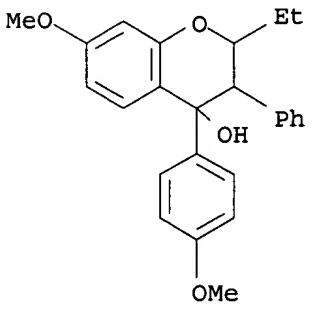
GI For diagram(s), see printed CA Issue.

AB The title compds. are prepd. by condensation of 3-aryl-4-chromanones with organo-metallic compds. followed by dehydration. A soln. of 0.66 g. I (R = R1 = H) (IV) in 30 ml. abs. C6H6 is dropped to a soln. of p-MeOC6H4MgBr (from 2.2 g. p-MeOC6H4Br and 0.23 g. Mg) in abs. Et2O, the Et2O distd., and the mixt. refluxed 16 hrs., cooled, decompd. with 100 ml. 10% HCl, and the C6H6 layer sped. to yield II (R = R1 = H,R2 = MeO), m. 144-5.degree. (CHCl3-Et2O). Likewise, the following II are prepd. (R, R1, R2, and m.p. given): H, H, H, 127-31.degree. (V); Et, H, H, 121-3.degree.; H, MeO, H, 151-2.degree.; Et, MeO, H, 158.degree. and 105.degree. (2 isomers); Et, MeO, MeO, 105-6.degree.; H, H, PhCH2O, 122-3.degree. (VI); Et, MeO, PhCH2O, 126.degree. and 137.degree. (2 isomers). To a soln. of IV (0.68 g.) in 30 ml. abs. C6H6 is added dropwise a soln. of PhLi (4 millimoles) in Et2O. After the same treatment as above V is isolated; when the mixt. is heated 5 hrs. after adding 10% HCl, III (R = R1 = R2 = H) is obtained, m. 130-2.degree. (Et2O-petroleum ether). Similarly prepd. are III (R = R1 = H, R2 = MeO), m. 119-21.degree., and III (R = H, R1 = R2 = MeO), m. 162-5.degree.. By treating I [R = H, R1 = tetrahydropyranyl-2-oxy (Q)] with PhMgBr as described, but decompg. with NH4Cl soln., II (R = R2 = H, R1 = Q) is obtained, while from the alk. washing fluid some II (R = R2 = H, R1 = OH) (VIII) is isolated). Similarly is prepd. from IV and p-QC6H4MgBr II (R = R1 = H, R2 = Q) (IX). VII (2 g.) is refluxed 2.5 hrs. in 50 ml. 5% HCl in dil. EtOH, the mixt. cooled and extd. with CHCl3 to yield III (R = R2 = H, R1 = OH) (X); similarly are obtained III (R = R1 = H, R2 = OH) (XI), m. 188-9.degree., from IX, and III (R = H, R1 = MeO, R2 = OH), m. 118.degree.. A soln. of 2 g. VI in 200 ml. EtOAc is hydrogenated at room temp. over 5% Pd-C, filtered, concd., the residue chromatographed on SiO2, and eluted with C6H6 to yield II (R = R1 = H, R2 = OH) (XII); similarly are prepd. II (R = H, R1 = MeO, R2 = OH), m.

173.degree. and II (R = Et, R1 = MeO, R2 = OH), m. 112.degree. and 150-2.degree. (2 isomers). XII (0.99 g.) is heated 5 hrs. at 100.degree. with a mixt. of 0.7 ml. H2SO4 and 13 ml. dioxane, cooled, poured on ice, extd. with CHCl3, the ext. concd., and the residue crystd. from Et2O-petroleum ether to give XI, m. 188-9.degree.. X (0.5 g.) in 10 ml. Me2CO is boiled 24 hrs. in N with 0.3 g. ClCH2CO2Et and 0.35 g. anhyd. K2CO3, concd., and extd. with CH2Cl2 to yield III (R = R2 = H, R1 = EtO2CCH2O) (XIII). XI (1 g.), 4 g. 2-pyrrolidinonethyl chloride, 1.2 g. dry K2CO3, and 40 ml. abs. Me2CO are stirred and boiled 20 hrs., concd., the residue dild. with H2O and Et2O, the Et2O layer sepd. dried, on KOH, concd., and the residue chromatographed on Al2O3 and eluted with CHCl3 to give III (R = R1 = H, R2 = 2-pyrrolidinoethoxy), m. 98-9.degree. (Me2CO-Et2O). X (1 g.), 5 ml. C5H5N, and 5 ml. Ac2O are heated 5 hrs. at 50.degree., cooled, and extd. with CHCl3 to yield III (R = R2 = H, R1 = AcO). To a soln. of 21 ml. POCl3 in 210 ml. abs. C5H5N is added with stirring in 15 min. at 5.degree. a soln. of 7.8 g. X in 105 ml. C5H5N; after 15 hrs. at room temp. the mixt. is poured on a mixt. of 3 kg. ice and 300 ml. concd. HCl, heated at 100.degree. for 90 min., cooled, extd. with EtOAc, the ext. washed with HCl, dried on Na2SO4, filtered, and concd. to yield the phosphate of X. H2NSO3H (6 g.) and 7.5 g. X are suspended in 5 ml. abs. C5H5N, stirred 90 min. at 100.degree., cooled, filtered, the filter washed with C5H5N, the filtrate extd. with abs. Et2O, the residue dried in vacuo, 75 ml. 12% NaOH and 53 ml. C5H5N added and shaken for 5 min.; the upper C5H5N layer washed with Et2O, MeOH added and concd., and the residue crystd. from MeOH to yield III (R = R2 = H, R1 = OSO3Na). XIII (2 g.) is refluxed 3 hrs. with 30 ml. 2N KOH in EtOH, and the soln. acidified to yield III (R = R2 = H, R1 = HO2CCH2O); XIII (3.5 g.) is refluxed 6 hrs. in a mixt. of 2 g. pyrrolidine and 10 ml. abs. C6H6, and the soln. concd. to yield III (R = R2 = H, R1 = QCOCH2O) (Q = pyrrolidino). II and III have antigonadotropic and contraceptive effects.

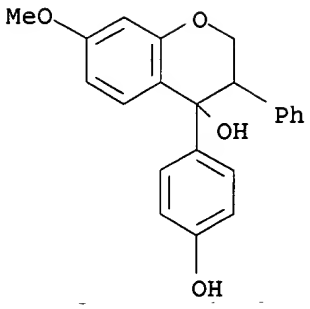
IT **13417-66-8P 13417-74-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

RN 13417-66-8 CAPLUS
CN 4-Chromanol, 2-ethyl-7-methoxy-4-(p-methoxyphenyl)-3-phenyl- (8CI) (CA INDEX NAME)



RN 13417-74-8 CAPLUS
CN 4-Chromanol, 4-(p-hydroxyphenyl)-7-methoxy-3-phenyl- (8CI) (CA INDEX NAME)

Golam Shameem



=> d ibib abs hitstr l7 tot

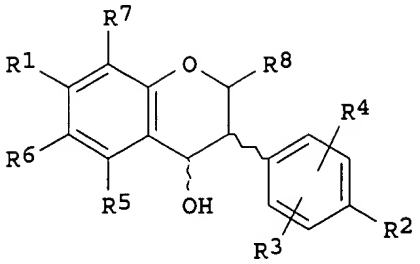
L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:592710 CAPLUS
DOCUMENT NUMBER: 133:177059
TITLE: Preparation of isoflavone derivatives
INVENTOR(S): Heaton, Andrew; Kumar, Naresh
PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000049009	A1	20000824	WO 2000-AU103	20000215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000008222	A	20011030	BR 2000-8222	20000215
EP 1153020	A1	20011114	EP 2000-904727	20000215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
NO 2001003945	A	20010814	NO 2001-3945	20010814

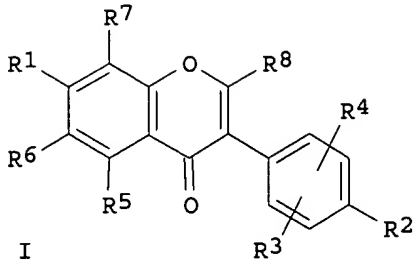
PRIORITY APPLN. INFO.: AU 1999-8685 A 19990215
WO 2000-AU103 W 20000215

OTHER SOURCE(S): MARPAT 133:177059
GI

Golam Shameem



I



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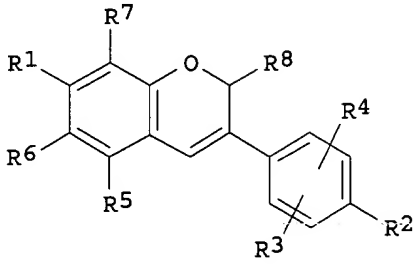


III

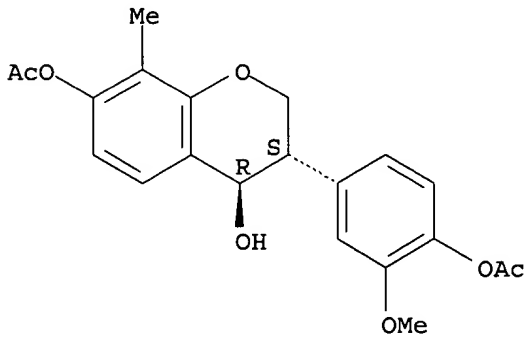
AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH2, NO2, alkyl, haloalkyl, aryl, arylalkyl,alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prepd. Thus, daidzein diacetate was prepd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the **hydrogenation** of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

IT **288266-89-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **288266-88-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

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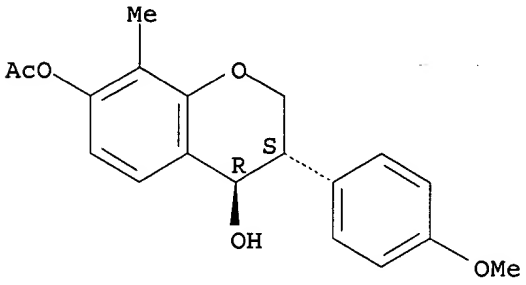
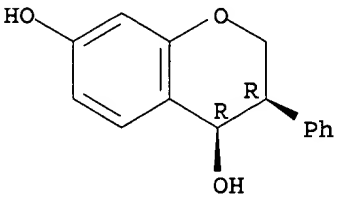
BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(prepn. of isoflavone derivs.)
RN 288266-88-6 CAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



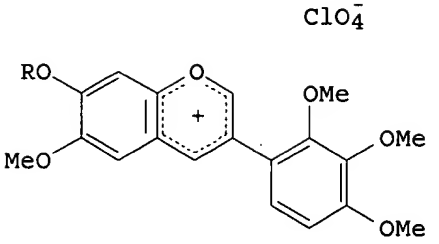
IT **288267-21-0P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of isoflavone derivs.)
RN 288267-21-0 CAPLUS
CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:148589 CAPLUS
DOCUMENT NUMBER: 104:148589
TITLE: The chemistry of the 'insoluble red woods'. Part 16. Some further observations on the condensation of isoflavylium salts with 1,3-diphenylpropenes
AUTHOR(S): Afonya, Theophilus C. A.; Epelle, Faithwin B. M.; Osman, Soad A. A.; Whalley, W. Basil
CORPORATE SOURCE: Sch. Pharm., London, WC1N 1AX, UK
SOURCE: J. Chem. Res., Synop. (1985), (10), 305
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:148589
GI



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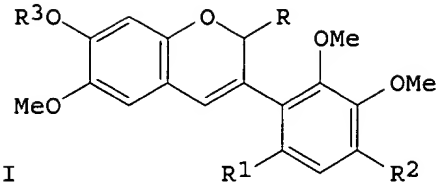
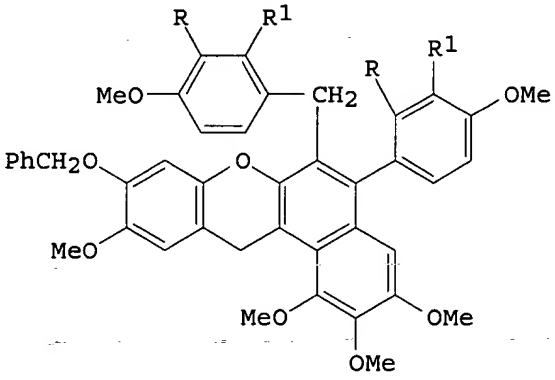


IV



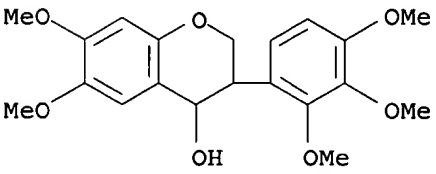
V

AB Condensation of isoflavylium perchlorate I (R = CH2Ph) (II) with 3,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-2,4 (III) in refluxing MeCN for 3 h gave isoflavene IV (R = R1 = H, R2 = OMe, R3 = CH2Ph) and benzoxanthene V (R = H, R1 = OMe). Similar reaction of II with 2,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-3,4 (VI) gave isoflavene IV (R = R2 = OMe, R1 = H; R = R2 = H, R1 = OMe; R3 = CH2Ph) and benzoxanthene V (R = OMe, R1 = H). Analogous reaction of I (R = Me) with III or VI gave only the isoflavene IV (R = R2 = OMe, R1 = H, R3 = Me). The prepns. of the starting materials are reported.

IT **100753-48-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and elimination reaction of, isoflavylium salt by)

RN 100753-48-8 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-6,7-dimethoxy-3-(2,3,4-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	47.95	49.32

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.58	-5.58

STN INTERNATIONAL LOGOFF AT 09:38:09 ON 13 AUG 2002

130

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1626gms

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 09	JAPIO to be reloaded August 18, 2002

NEWS EXPRESS	February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * *

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FILE 'HOME' ENTERED AT 10:34:54 ON 13 AUG 2002

=> s flavone
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:35:30 ON 13 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3
DICTIONARY FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s flavone
6194 FLAVONE
1 FLAVONES
L1 6194 FLAVONE
(FLAVONE OR FLAVONES)

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.38	4.59

FILE 'CAPLUS' ENTERED AT 10:35:54 ON 13 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 13 Aug 2002 VOL 137 ISS 7
FILE LAST UPDATED: 12 Aug 2002 (20020812/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

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L2        28254 L1

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L3         1943 L1/PROC
                (L1 (L) PROC/RL)

=> s l1/prep
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        2897488 PREP/RL
L4         3978 L1/PREP
                (L1 (L) PREP/RL)

=> s l3 and hydrogenation?
      148247 HYDROGENATION?
L5           3 L3 AND HYDROGENATION?

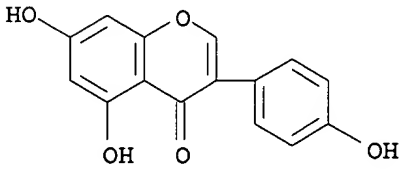
=> d ibib abs hitstr l5 tot

L5   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:         1995:787564  CAPLUS
DOCUMENT NUMBER:          123:226958
TITLE:                    A urinary profile study of dietary phytoestrogens. The
                          identification and mode of metabolism of new
                          isoflavonoids
AUTHOR(S):                Joannou, G. E.; Kelly, G. E.; Reeder, A. Y.; Waring,
                          M.; Nelson, C.
CORPORATE SOURCE:         Department of Metabolic Mass Spectrometry, Royal
                          Prince Alfred Hospital, Sydney, 2050, Australia
SOURCE:                   J. Steroid Biochem. Mol. Biol. (1995), 54(3/4), 167-84
                          CODEN: JSBBEZ; ISSN: 0960-0760
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   The metabolic fate of the dietary isoflavones daidzein and genistein was
     investigated in human volunteers challenged with soya. Urinary diphenols,
     isolated by partition chromatog. on Sephadex LH-20, were characterized and
     identified by profile capillary gas chromatog. (GC) and electron
     ionization mass spectrometry (GC-EIMS) anal. of the trimethylsilyl ether
     (TMS) derivs. Novel isoflavonic phytoestrogens found in the urine of
     volunteers were those of tetrahydrodaidzein, dihydrogenistein,
     6'-hydroxy-O-demethylangolensin and 2-dehydro-O-demethylangolensin. Other
     known diphenols identified were those of equol, dihydrodaidzein,
     O-demethylangolensin, daidzein, genistein, glycitein, and the lignan
     enterolactone. Two other urinary isomers with a fragmentation pattern
```

closely resembling that of the persilylated TMS ethers of cis/trans-isomers of tetrahydrodaidzein, were characterized based on the elucidation of fragments assocd. with the loss of a nonphenolic-OTMS functional group in ring-C. These are fragments presented in the persilylated mass spectra of isoflavan-4-ols and isoflav-3-ene-4-ols, demonstrated here by a combination of simple and tandem mass spectrometry study of the deuterated persilylated TMS ethers of dihydrodaidzein. In a similar study the authors also present the data on the structural identification and fragment elucidation of the keto/enol tautomers of the TMS ether derivs. of the dihydro derivs. of daidzein and genistein, obsd. in the urine of volunteers and considered probable products of the derivatization process. Finally, the GC and GC-MS data of two unknown isoflavonoids and that of a lignan-like compd. are presented together with those of dihydrodaidzein, dihydrogenistein, tetrahydrodaidzein and 2-dehydro-O-demethylangolensin. The latter four were obtained here as products of small scale chem. synthesis in a preliminary study on the tentative identification of urinary isoflavonoids in human volunteers challenged with soya.

IT **446-72-0**, Genistein **486-66-8**, Daidzein
RL: BPR (Biological process); RCT (Reactant); BIOL (Biological study); **PROC (Process)**
(metabolic fate of human dietary isoflavones and **hydrogenation** of)

RN 446-72-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 486-66-8 CAPLUS
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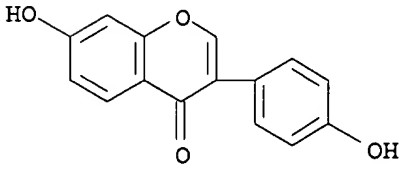
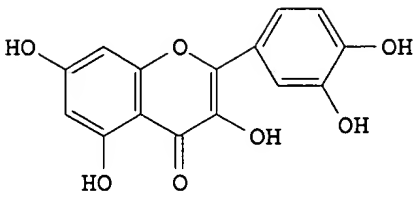


L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:605536 CAPLUS
DOCUMENT NUMBER: 99:205536
TITLE: Studies on drug metabolism by use of isotopes. XXVII: Urinary metabolites of rutin in rats and the role of intestinal microflora in the metabolism of rutin
AUTHOR(S): Baba, Shigeo; Furuta, Takashi; Fujioka, Minoru; Goromaru, Tsuyoshi
CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan

Golam Shameem

SOURCE: J. Pharm. Sci. (1983), 72(10), 1155-8
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

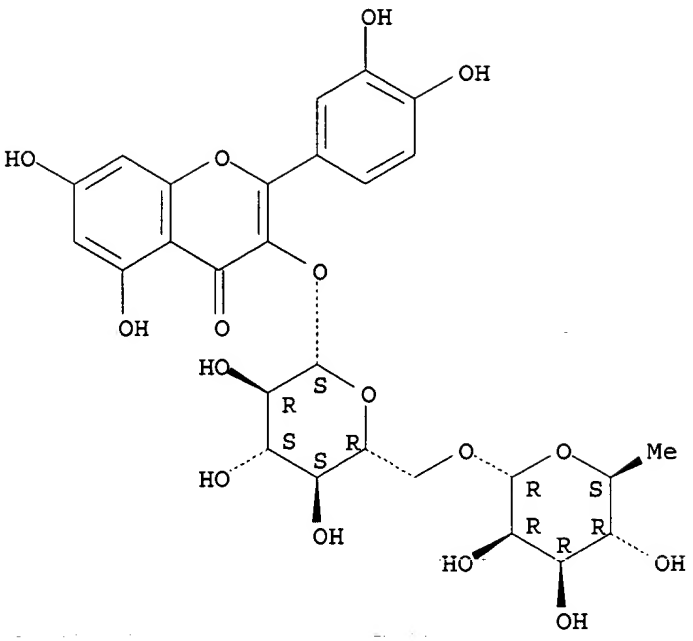
AB Anal. of urinary metabolites of orally administered rutin (I) [153-18-4] labeled with deuterium ([2',5',6'-2H]rutin (rutin-d) [78800-17-6]) was carried out by gas-liq chromatog.-mass spectroscopy. In rat urine, 3-hydroxyphenylacetic acid [621-37-4], 3-methoxy-4-hydroxyphenylacetatic acid [34919-76-1] 3,4-dihydroxyphenylacetic acid [102-32-9], 3,4-dihydroxytoluene [452-86-8], and 3-(m-hydroxyphenyl)propionic cid [621-54-5] were identified as rutin metabolites and were differentiated from the corresponding endogeneous compds. Unchanged I and quercetin [117-39-5] were not present in the urine. Rutin-d was injected i.p. in rats, administered orally to neomycin-treated rats, and incubated in vitro with the intestinal contents of rats. The expts. suggested the involvement of intestinal microflora in the metab. of orally administered I.

IT **153-18-4**
RL: BPR (Biological process); BIOL (Biological study); **PROC (Process)**
(metab. of, intestinal microorganisms in)

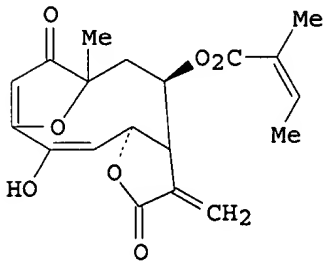
RN 153-18-4 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-[[6-O-(6-deoxy-.alpha.-L-mannopyranosyl)-.beta.-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:140446 CAPLUS
DOCUMENT NUMBER: 92:140446
TITLE: Some derivatives of budlein A and B and the cytotoxic activity of substance A in two cell lines
AUTHOR(S): Roche, P.; Rosas, N.; Taboada, J.; Gonzalez Diddi, M.; Tellez, J.
CORPORATE SOURCE: Inst. Quim., Univ. Nac. Auton. Mexico, Mexico City, 20, Mex.
SOURCE: Rev. Latinoam. Quim. (1979), 10(4), 145-9
CODEN: RLAQA8; ISSN: 0370-5943
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
GI



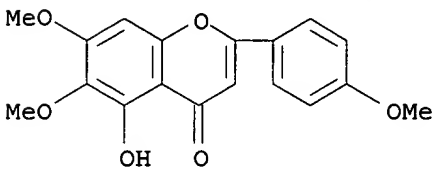
I

AB Budlein A (I) [59481-48-0], budlein B [60147-79-7], and salvigenin [19103-54-9] were isolated from Viguiera plants. Some derivs. of I (Me ether, chlorinated and hydrogenated products) and budlein B (Cope rearrangement product) were prepd. and identified. The cytotoxic activity of only 1 of the compds. (I) was evaluated. At 1-10 .mu.g/mL, I only slightly decreased the no. of mitosis in HEp-2 cell cultures (human

laryngeal carcinoma), whereas at 50 .mu.g/mL it inhibited cellular growth by 79%. For murine connective tissue cultures, I inhibited cellular growth by 83% at 1 .mu.g/mL and increased the no. of multinuclear cells by .apprx.5-fold.

IT **19103-54-9**
RL: **PROC (Process)**
(isolation of, from Viguiera)

RN 19103-54-9 CAPLUS
CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

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          2454 ISOFLAVONES
L6         199 L3 AND ISOFLAVONES

=> s l6/proc
         28254 L1
       3189134 PROC/RL
          1943 L1/PROC
                  (L1 (L) PROC/RL)
             1 ISOFLAVONES/CT
       3189134 PROC/RL
             0 ISOFLAVONES/PROC
                  (ISOFLAVONES/CT (L) PROC/RL)
L7           0 ((L1/PROC) AND ISOFLAVONES/PROC)

=> s l6 and hydrogenation
        147967 HYDROGENATION
          1893 HYDROGENATIONS
        148239 HYDROGENATION
                  (HYDROGENATION OR HYDROGENATIONS)
L8           1 L6 AND HYDROGENATION

=> d ibib abs hitstr tot

L8   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:        1995:787564  CAPLUS
DOCUMENT NUMBER:         123:226958
TITLE:                   A urinary profile study of dietary phytoestrogens. The
                         identification and mode of metabolism of new
                         isoflavonoids
AUTHOR(S):               Joannou, G. E.; Kelly, G. E.; Reeder, A. Y.; Waring,
                         M.; Nelson, C.
CORPORATE SOURCE:        Department of Metabolic Mass Spectrometry, Royal
                         Prince Alfred Hospital, Sydney, 2050, Australia
SOURCE:                  J. Steroid Biochem. Mol. Biol. (1995), 54(3/4), 167-84
                         CODEN: JSBBEZ; ISSN: 0960-0760
DOCUMENT TYPE:           Journal
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Golam Shameem

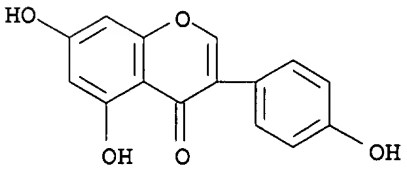
LANGUAGE: English

AB The metabolic fate of the dietary **isoflavones** daidzein and genistein was investigated in human volunteers challenged with soya. Urinary diphenols, isolated by partition chromatog. on Sephadex LH-20, were characterized and identified by profile capillary gas chromatog. (GC) and electron ionization mass spectrometry (GC-EIMS) anal. of the trimethylsilyl ether (TMS) derivs. Novel isoflavonic phytoestrogens found in the urine of volunteers were those of tetrahydrodaidzein, dihydrogenistein, 6'-hydroxy-O-demethylangolensin and 2-dehydro-O-demethylangolensin. Other known diphenols identified were those of equol, dihydrodaidzein, O-demethylangolensin, daidzein, genistein, glycitein, and the lignan enterolactone. Two other urinary isomers with a fragmentation pattern closely resembling that of the persilylated TMS ethers of cis/trans-isomers of tetrahydrodaidzein, were characterized based on the elucidation of fragments assocd. with the loss of a nonphenolic-OTMS functional group in ring-C. These are fragments presented in the persilylated mass spectra of isoflavan-4-ols and isoflav-3-ene-4-ols, demonstrated here by a combination of simple and tandem mass spectrometry study of the deuterated persilylated TMS ethers of dihydrodaidzein. In a similar study the authors also present the data on the structural identification and fragment elucidation of the keto/enol tautomers of the TMS ether derivs. of the dihydro derivs. of daidzein and genistein, obsd. in the urine of volunteers and considered probable products of the derivatization process. Finally, the GC and GC-MS data of two unknown isoflavonoids and that of a lignan-like compd. are presented together with those of dihydrodaidzein, dihydrogenistein, tetrahydrodaidzein and 2-dehydro-O-demethylangolensin. The latter four were obtained here as products of small scale chem. synthesis in a preliminary study on the tentative identification of urinary isoflavonoids in human volunteers challenged with soya.

IT **446-72-0**, Genistein **486-66-8**, Daidzein
RL: BPR (Biological process); RCT (Reactant); BIOL (Biological study); **PROC (Process)**
(metabolic fate of human dietary **isoflavones** and **hydrogenation** of)

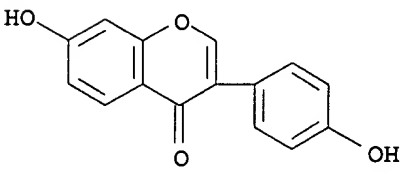
RN 446-72-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

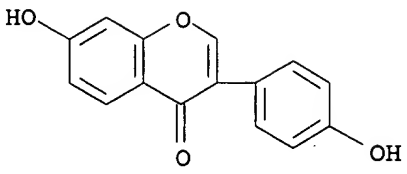


RN 486-66-8 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



Golam Shameem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